Skoltech
Skolkovo Institute of Science and Technology

Jury Member Report – Doctor of Philosophy thesis.

Name of Candidate: Christian Tantardini

PhD Program: Materials Science and Engineering

Title of Thesis: A study of chemical bonding through quantum chemical topology

Supervisor: Prof. Artem Oganov

Date of Thesis Defense: 31 January 2020

Name of the Reviewer: Professor Xavier Assfeld

I confirm the absence of any conflict of interest (Alternatively, Reviewer can formulate a possible conflict)	**Signature:**  UMR CNRS/UL 7019 - LPCT P<sr Xavier ASSFELD, Directeur Université de Lorraine Faculté des Sciences et Technologies Campus aiguillettes - BP 70239 54500 VANDŒUVRE LES NANCY **Date: December 11th 2019**

The purpose of this report is to obtain an independent review from the members of PhD defense Jury before the thesis defense. The members of PhD defense Jury are asked to submit signed copy of the report at least 30 days prior the thesis defense. The Reviewers are asked to bring a copy of the completed report to the thesis defense and to discuss the contents of each report with each other before the thesis defense.

If the reviewers have any queries about the thesis which they wish to raise in advance, please contact the Chair of the Jury.

Reviewer's Report

Reviewers report should contain the following items:

- Brief evaluation of the thesis quality and overall structure of the dissertation.
- The relevance of the topic of dissertation work to its actual content
- The relevance of the methods used in the dissertation
- The scientific significance of the results obtained and their compliance with the international level and current state of the art
- The relevance of the obtained results to applications (if applicable)
- The quality of publications

The summary of issues to be addressed before/during the thesis defense

The manuscript presented by C. Tantardini in order to obtain his Ph.D. diploma is divided in four chapters containing the results obtained during the past years. It starts with a general introduction which explains the theoretical background needed by the reader to fully appreciate the work done. Mainly QTAIM (Quantum Theory of Atoms In Molecule) is detailed with several variants. This part is quite complete and the related bibliography is correctly addressed. The first three chapters containing the results are all based on papers published in international peer-reviewed journals. They contain a short summary and the published article(s). Only the fourth chapter presents data that are not published yet. It deals with determining Pauling's electronegativity for chemical elements under high pressure. Finally, the manuscript ends with a general conclusion.

Eleven papers have been published by the candidate in good journals (TCA, JCC, PCCP, …). This is very impressive and it shows how relevant and important the researches conducted by C. Tantardini are. What is also even more impressive is the number of different treated subjects which extend from defining a new equation of state to the chemical reactivity of organic molecules. It is very rare to find Ph.D. candidates that are able to tackle such diversity.

If I were to ask for modifications prior the thesis defense, I would ask to enhance a little bit the fourth chapter with references on these new phenomena induced by very high pressure. It is also not perfectly clear to me how the different values of the external pressure are fixed by the simulation protocol.

Overall, albeit some grammatical polishing should be done, the manuscript is acceptable for the defense and corresponds largely to the international standards to obtain a Ph.D. I therefore recommend it for defense.

Provisional Recommendation

☒ *I recommend that the candidate should defend the thesis by means of a formal thesis defense*

☐ *I recommend that the candidate should defend the thesis by means of a formal thesis defense only after appropriate changes would be introduced in candidate's thesis according to the recommendations of the present report*

☐ *The thesis is not acceptable and I recommend that the candidate be exempt from the formal thesis defense*